Possible explanation for the absence of bilayer splitting in YBCO

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It has been claimed that the absence of the bilayer splitting in the high-temperature superconductor YBCO is a strong experimental indication that there are no coherent quasiparticles present in the CuO planes[1]. We study a pair of strongly correlated planes which are connected by a hopping transfer integral $t_\perp$ in the limit of large in-plane coordination number. The effect of the correlation is incorporated in a dynamical mean-field theory, where the Weiss field is determined by a two-site Hubbard Hamiltonian. We have solved this problem by numerical techniques and present results for the spectral function ρ for relevant parameters of the model. For small $t_\perp$ we find the coherent hoping between planes to be proportional to the in-plane quasiparticle renormalisation.

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The transport properties of the high temperature superconductors show an unusual behavior in many respects. Anderson[1] has emphasized the difference between the transport properties in a CuO plane and perpendicular to the CuO plane stressing in particular the optical conductivity, in the c-direction perpendicular to the CuO planes[2]. Also photoemission experiments[3,4] in YBCO show only a small if any splitting of the bonding and antibonding CuO plane bands due to coherent hopping between the CuO planes. This is even more surprising in view of the relatively large value of the bare hopping matrix element, $t_\perp \approx 0.3\,\mathrm{eV}$ compared to $t_\parallel \approx 1\,\mathrm{eV}$, estimated from bandstructure calculations[5]. The experimental data have been interpreted as a signal for the absence of coherent quasiholes in the CuO plane[1].

The question of how interactions affect the coherent transport between the planes has been studied mostly on one dimensional strongly correlated systems because in that case it is clear that the excitations above the ground state are spinons and holons as in the original proposal by Anderson. Two coupled chains (ladders) have been recently studied in detail by many groups with numerical and analytic techniques[6,7,8,9,10,11]. The result was that the hopping matrix element $t_\perp$ is a relevant perturbation for physically relevant values of the Luttinger liquid exponents and that the transport between the chains is coherent. Recently it has been claimed from an exact diagonalization study that for longer range interactions in the chains the coherent hopping between the chains can be reduced to zero for a finite value of the bare hopping matrix element $t_\perp$[12].

The problem of two coupled CuO planes is clearly more difficult since at this point the ground state and the excitation spectrum even for a single plane of the two dimensional Hubbard model away from half filling are not known. The problem has been studied with numerical techniques like Quantum Monte Carlo (QMC)[13] and the fluctuation exchange approximation (FLEX) approximation[14,15,16]. The subtle features of the dynamics of the quasiparticles in the coupled planes can currently not be resolved in the QMC due to finite size effects although the results for one plane look encouraging[9]. The FLEX calculations[14,15,16] are able to resolve the dynamics and yield surprisingly good results when compared to the QMC calculation but this approximation is uncontrolled in the regime where the interaction is large.

In this paper we present a calculation of the spectral function and the reduction of the coherent hopping in an approximation where the local correlations are taken into account exactly. We are in particular interested in the dynamics of the quasiparticles. We consider a model of two strongly correlated planes. We neglect the Coulomb interaction between the two planes. The motion of the holes in each plane is described by a Hubbard Hamiltonian.

$$H_a = -t \sum_{<ij>\sigma} c^\dagger_{ai\sigma} c_{aj\sigma} - \mu \sum_{i\sigma} n_{ai\sigma} + U \sum_i n_{ai\uparrow} n_{ai\downarrow}, \tag{1}$$

where t is the hopping matrix element between two nearest neighbors i and j, μ is the chemical potential, $c^\dagger_{ai\sigma}$ is the electron creation operator on site i with spin σ in plane a ($a = 1, 2$) and $n_{ai\sigma}$ is the electron number operator for spin σ at site i in plane a, $n_{ai\sigma} = c^\dagger_{ai\sigma} c_{ai\sigma}$. We denote the electron creation and annihilation operators in plane 1 by $c^\dagger_{1i}$ and c_{1i} respectively and in plane 2 by $c^\dagger_{2i}$ and c_{2i}. The two planes are coupled by the hopping

term

$$H_{12} = -t_\perp \sum_{i\sigma} \left(c^\dagger_{1i\sigma} c_{2i\sigma} + c^\dagger_{2i\sigma} c_{1i\sigma} \right) \quad (2)$$

with the hopping matrix element $t_\perp$ connecting site i in plane 1 with site i in plane 2. The complete Hamiltonian for the bilayer is then $H = H_1 + H_2 + H_{12}$. An exact solution of this problem at this point in time is clearly impossible since already H_1 and H_2 cannot be treated exactly in two spatial dimensions. However some progress can be made by introducing the so called dynamical mean field approximation in which the local correlations are treated exactly. For a review of this method see e.g.[17,18]. The important point is that the dynamics of the quasiparticles hopping onto a given site and leaving a given site is kept. To apply this approximation to the problem at hand the number of neighbors z of each site in a given plane $(1, 2)$ to its neighbors in the *same* plane has to go to infinity, see Fig. 1. In this approach the phase information of the electrons hopping from a site j to a given site i in the same plane is lost because the phase information is averaged of over the large number of sites j connected to i. The hopping term between the planes has to be treated separately because there is only one site in plane 2 connected to a given site in the plane 1.

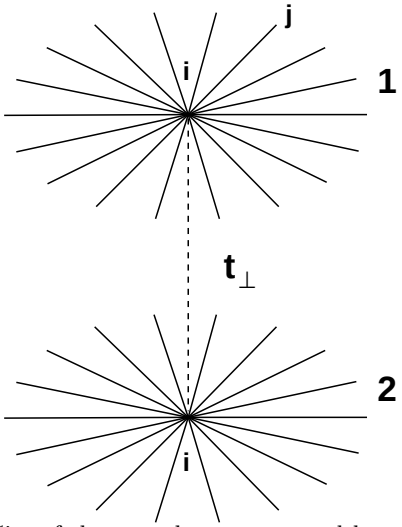

FIG. 1. Site of the two planes connected by nonzero hopping matrix elements

The non interacting ($U = 0$) Green's function $\boldsymbol{G}_0^{-1}$ is defined as $[\boldsymbol{G}_0(k,\tau)]_{aa'} = -<T_\tau c_{ak\alpha}(\tau) c^\dagger_{a'k\beta}(0)>$ with $a, a' \in \{1, 2\}$. It is given by

$$\boldsymbol{G}_0^{-1}(k,\omega) = \omega - \boldsymbol{H}(U=0) = \begin{bmatrix} \omega - \epsilon_k & t_\perp \\ t_\perp & \omega - \epsilon_k \end{bmatrix} \quad (3)$$

In the paramagnetic phase the self energy $\boldsymbol{\Sigma}(k,\omega)$ has only two independent components. We denote them by $\Sigma_\parallel$ and $\Sigma_\perp$ in the present basis

$$\boldsymbol{\Sigma} = \begin{bmatrix} \Sigma_\parallel & \Sigma_\perp \\ \Sigma_\perp & \Sigma_\parallel \end{bmatrix} \quad (4)$$

The Hamiltonian is diagonal in the bonding - antibonding representation. The full Green's function can be obtained from the Dyson equation

$$\boldsymbol{G}^{-1}(k,\omega) = \boldsymbol{G}_0^{-1}(k,\omega) - \boldsymbol{\Sigma}(k,\omega) \quad (5)$$

We are now in the position to derive the dynamical mean field equations for the coupled planes. In the limit of large coordination number the self energy becomes local and therefore k-independent[19]. The only k-dependence of the Green's function is left in the free electron dispersion ϵ_k. This k-dependence can be absorbed in the density of states $D(\epsilon) = \sum_k \delta(\epsilon - \epsilon_k)$, which of course depends on the type of lattice in which the electrons are moving. For the hypercubic lattice $D(\epsilon) = exp(-(\epsilon/\sqrt{2}t)^2)/t\sqrt{2\pi}$. The full *local* Green's function is therefore given by:

$$\boldsymbol{G}(\omega) = \int d\epsilon_{\mathbf{k}} D(\epsilon_{\mathbf{k}}) \left(\boldsymbol{\mathcal{G}}_0^{-1}(\epsilon,\omega) - \boldsymbol{\Sigma}(\omega) \right)^{-1} \quad (6)$$

In the dynamical mean field approach $\boldsymbol{\mathcal{G}}_0^{-1}(\tau)$ plays the role of a Weiss field. The main point of this approach is that the *local* self energy of the full problem is determined by the local impurity model[20]: in our case a two impurity model. It has the action

$$S = \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma \bar{\psi}_\sigma(\tau) \boldsymbol{\mathcal{G}}_0^{-1}(\tau - \tau') \psi_\sigma(\tau') + U \sum_{a=1,2} \int_0^\beta d\tau \; \bar{\psi}_{a\uparrow}(\tau) \psi_{a\uparrow}(\tau) \bar{\psi}_{a\downarrow}(\tau) \psi_{a\downarrow}(\tau) \quad (7)$$

where $\bar{\psi}_\sigma = (\bar{\psi}_{1\sigma}, \bar{\psi}_{2\sigma})$ is a spinor of Grassmann variables. We only consider the paramagnetic state. The Weiss field $\boldsymbol{\mathcal{G}}_0^{-1}(\omega)$ is therefore diagonal in spin space. Using Eq. 6 we obtain the full local Green's function in the bonding, anti-bonding basis:

$$\boldsymbol{G}(\omega) = \begin{bmatrix} \tilde{D}_+(\omega) & 0 \\ 0 & \tilde{D}_-(\omega) \end{bmatrix} \quad (8)$$

where $\tilde{D}_\pm(\omega) = \tilde{D}(\omega - \Sigma_\parallel(\omega) \pm (t_\perp - \Sigma_\perp(\omega)))$ is the Green's function of the anti-bonding and bonding band respectively and

$$\tilde{D}(\omega) = \int d\epsilon \frac{D(\epsilon)}{\epsilon - \omega} \quad (9)$$

is the Hilbert transform of the density of states $D(\epsilon)$.

We solve the two impurity model, Eq. 7, using the "iterated perturbation theory" (IPT)[21] which has been shown to yield qualitative agreement with QMC and exact diagonalization approaches for interaction strength up to $U/t \sim 4$. The self energy is approximated by the first two terms of a perturbation expansion in the interaction U. However these two terms are calculated with the local Green's function $\mathcal{G}_0$ which is then determined selfconsistently. For doping levels away from half filling we used an extension of the IPT due to Kajueter and Kotliar[22].

In Fig. 2 the spectral functions of the bonding and antibonding band are shown as a function of frequency for a $U = 4$, a bilayer hopping of $t_\perp = 0.3$ and a filling of $n = 0.4375$. All energies are measured in units of the in-plane hopping matrix element t. For each band the

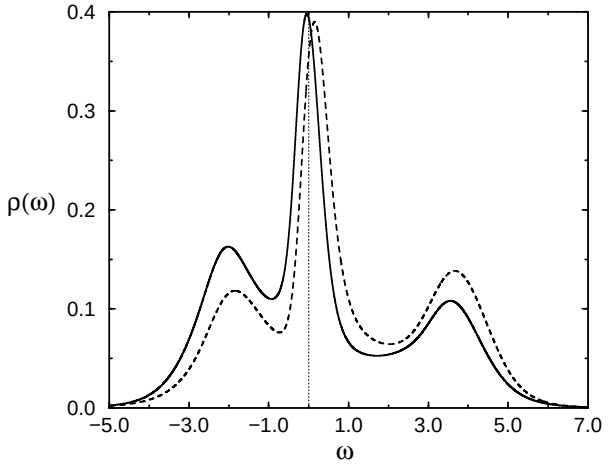

FIG. 2. Spectral functions for the bonding (solid line) and anti-bonding (dashed line) band. The parameters are $U = 4$, $n = 0.4375$ and $t_\perp = 0.3$. The dotted vertical line marks the Fermi energy.

lower and upper Hubbard band can be clearly identified. The quasiparticle peak close to $\omega = 0$ for each band is slightly shifted away from zero as expected from the noninteracting limit. The first interesting observation is that the spectral weight in the lower and the upper Hubbard band is not symmetric anymore even at half filling. The spectral density of the upper Hubbard band of the bonding band and the lower Hubbard band of the anti-bonding band are suppressed. With increasing hopping between the planes the quasiparticle peaks move further apart and the features associated with the Hubbard bands become less and less pronounced. For very large values of $t_\perp$ the noninteracting density of states of the two bands is recovered. The small features in the spectral function which are associated with the formation of so called shadow bands as obtained in the FLEX calculation[15] can not be found in our calculation, because the finite momentum antiferromagnetic fluctuations are missing from our calculation. However the redistribution of weight from the Hubbard bands to the quasiparticle peak and vice versa has not been resolved in the FLEX perhaps because it is inherently a weak coupling approach. At half filling both bands are filled up to $\omega = 0$. The self energy of the bonding and antibonding propagator is given by $\Sigma_\parallel(\omega) \pm \Sigma_\perp(\omega)$. For small values of $t_\perp$ the quasiparticle weight is strongly reduced.

Next we discuss the reduction of the coherent hopping between the planes. There are two measures of coherent hopping: one is ΔE, the splitting in frequency between the quasiparticle peaks in the bonding and anti-

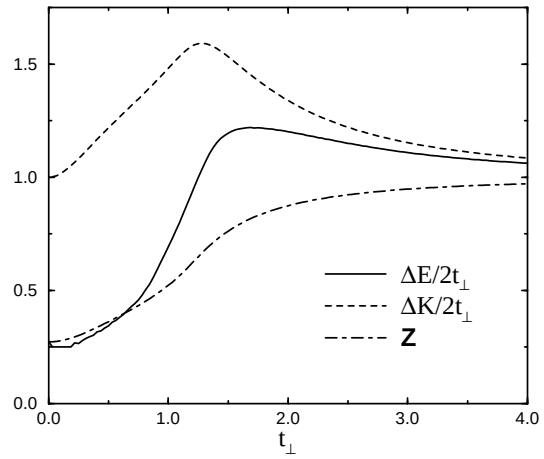

FIG. 3. The splitting $\Delta E/2t_\perp$ ($\Delta K/2t_\perp$) of the coherent hopping between planes as a function of $t_\perp$. The parameters are $U = 4$ and $n = 0.5$. The dashed line refers to the splitting in energy, the solid line to the splitting in ϵ_k. The spectral weight of the quasiparticle peaks is shown as dashed-dotted line.

bonding bands; the other is $\Delta K = 2(t_\perp - \Sigma_\perp(\omega = 0))$, the splitting in momentum space between the bonding and antibonding bands at the Fermi surface. We consider $\Delta E/2t_\perp$ first. Its $t_\perp$ dependence is shown in Fig. 3. In the noninteracting case ΔE assumes the value $2t_\perp$. For small $t_\perp$ the ratio $\Delta E/2t_\perp$ is clearly reduced from the noninteracting value of 1. However unless one drives the system through the Mott transition at very large values of U where the planes themselves are insulating the reduction factor is nonzero. In the $t_\perp \to 0$ limit the reduction factor can be analytically related to the reduction of the bandwith in the plane. The off-diagonal part of the self-energy $\Sigma_\perp$ is proportional to $t_\perp^3$ for small $t_\perp$. The position of the quasiparticle-peak is given by the poles of $\tilde{D}_\pm(z)$ in the complex plane. For small $t_\perp$ and doping not too far from half filling the position of the pole is given by the zero of $\omega - \mathrm{Re}\ \Sigma_\parallel(\omega) \pm t_\perp + O(t_\perp^3) = 0$. The selfenergy does not depend on the momentum. The reduction of the bandwidth is therefore solely given by $(1 - \partial\Sigma_\parallel(\omega)/\partial\omega)^{-1}$ which is the same as the reduction of the bandwith due to interaction in a single plane. Interestingly the coherent hopping is seen to be enhanced for larger values of $t_\perp$. This effect can be understood in terms of a level repulsion of the two site Hubbard model in the regime where $t_\perp \gg U \gg t$. For very large values of $t_\perp$ the splitting asymptotically approaches the value $2t_\perp$ as one would expect from the noninteracting system.

In Fig. 4 we plotted the spectral density $A(\epsilon_k, \omega)$ at zero temperature as function of frequency for parameter values $t_\perp = 0.3$ and $U = 4$. The wavevector dependence is only implicitly contained via ϵ_k, because of the local nature of dynamical mean field theory. For ϵ_k close to zero we observe one sharp peak associated with the bond-

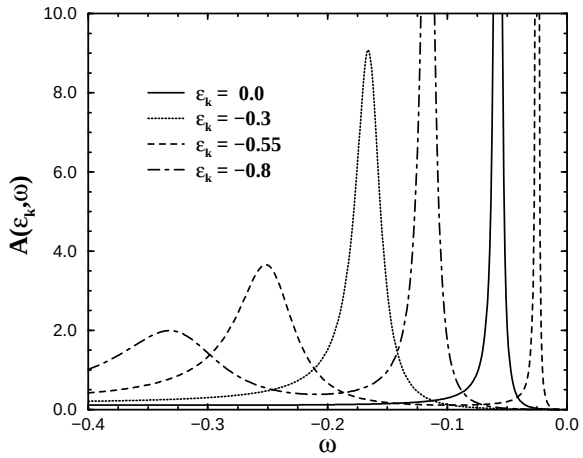

FIG. 4. Single particle spectral function $A(\epsilon_{\mathbf{k}}, \omega)$ vs. ω for different values of $\epsilon_{\mathbf{k}}$. The parameters are $t_\perp = 0.3$, $U = 4$ and $n = 0.4375$.

ing band just below the Fermi level as one would expect (The bonding band actually crosses the Fermi level at $\epsilon_{\mathbf{k}} \approx 0.15$). When going to lower energies this maximum moves downwards in the spectrum and very rapidly becomes broader. The broadening is due to strong correlations which manifest themself in a rapid increase of the self energy away from $\omega = 0$. For $\epsilon_k \approx -0.55$ a new sharp peak due to the antibonding band appears. The peak of the bonding band, however, is already rather broad at this energy. The splitting ΔK between the $\epsilon_{\mathbf{k}}$ values where the bonding and antibonding bands cross the Fermi surface is thus $\Delta K \approx 0.7$ so for these parameters $\Delta K/2t_\perp \approx 1.1$.

In conclusion we have studied the problem of two coupled planes in the dynamical mean field theory in the paramagnetic state as a function of interaction, doping and interplane hopping matrix elements. Within our approximation the coherent hopping between the planes is strongly reduced due to the interaction however it stays nonzero as long as the planes stay in the paramagnetic phase. It is still an open question if short range antiferromagnetic correlations which are completely neglected in our approach can suppress the coherence between coupled planes even further. For intermediate values of the interplane coupling the coherent hopping motion of the quasiparticles between planes is increased by the interaction. The spectral weight in the Hubbard bands is redistributed in an unsymmetric way even at half filling. Our approach can be easily extended to include more realistic density of states. It is interesting to examine the stability of other groundstates like for example the antiferromagnetic groundstate.

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